

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 1120 L/kg

Global applicability domain: Inside

Local applicability domain index: 4.55e-01

Confidence level: 5.60e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Fenarimol</div> <div>Measured: 603</div> <div>Predicted: 753</div>	<div>Image not found</div> <div>2,2'-Biquinoline</div> <div>Measured: 10500</div> <div>Predicted: 32700</div>	<div>Image not found</div> <div>Cinmethylin</div> <div>Measured: 398</div> <div>Predicted: 483</div>
<div>Image not found</div> <div>Cianidanol</div> <div>Measured: 107</div> <div>Predicted: 37.6</div>	<div>Image not found</div> <div>1-Amino-2-methylantraquinone</div> <div>Measured: 7940</div> <div>Predicted: 4960</div>	